Recent developments in affine symmetry principles for non-crystallographic systems

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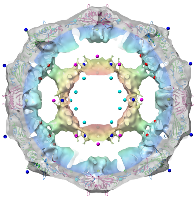
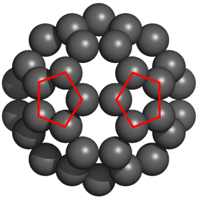
Overview

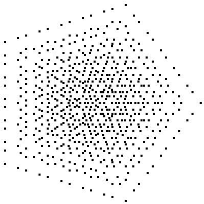
1. Affine extensions
   - Direct extensions
   - Induced extensions
2. Applications
   - Virus Structure
   - Fullerenes and Carbon onions
3. Conclusions

Motivation: Viruses

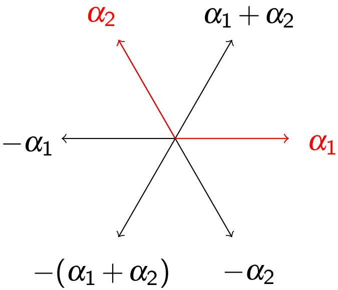
- Geometry of polyhedra described by Coxeter groups
- Viruses have to be 'economical' with their genes
- Encode structure modulo symmetry
- Largest discrete symmetry of space is the icosahedral group
- Many other 'maximally symmetric' objects in nature are also icosahedral: Fullerenes & Quasicrystals
- But: viruses are not just polyhedral – they have radial structure. Affine extensions give translations







Root systems – A_2



Root system Φ: set of vectors α such that $\boxed{\Phi \cap \mathbb{R}\alpha = \{-\alpha, \alpha\} \ \forall\, \alpha \in \Phi}$ and $\boxed{s_\alpha \Phi = \Phi \ \forall\, \alpha \in \Phi}$

Simple roots: express every element of Φ via a $\mathbb{Z}$-linear combination (with coefficients of the same sign).

Cartan Matrices

Cartan matrix of α_is is $\boxed{A_{ij} = 2\frac{(\alpha_i, \alpha_j)}{(\alpha_i, \alpha_i)} = 2\frac{|\alpha_j|}{|\alpha_i|}\cos\theta_{ij}}$

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angles $\boxed{\cos^2\theta_{ij} = \frac{1}{4}A_{ij}A_{ji}}$ lengths $\boxed{l_j^2 = \frac{A_{ij}}{A_{ji}}l_i^2}$

$\boxed{A_{ii} = 2}$ $\boxed{A_{ij} \in \mathbb{Z}^{\leq 0}}$ $\boxed{A_{ij} = 0 \Leftrightarrow A_{ji} = 0}$.

$$A_2\colon\; A = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

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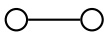
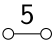
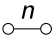
Coxeter-Dynkin diagrams: node = simple root, no link = roots orthogonal, simple link = roots at $\frac{\pi}{3}$, link with label m = angle $\frac{\pi}{m}$.

A_2  H_2 

$I_2(n)$ 

Coxeter groups

A Coxeter group is a group generated by some involutive generators $s_i, s_j \in S$ subject to relations of the form $\boxed{(s_i s_j)^{m_{ij}} = 1}$ with $m_{ij} = m_{ji} \geq 2$ for $i \neq j$.

The finite Coxeter groups have a geometric representation where the involutions are realised as reflections at hyperplanes through the origin in a Euclidean vector space $\mathscr{E}$. In particular, let $(\cdot|\cdot)$ denote the inner product in $\mathscr{E}$, and v, $\alpha \in \mathscr{E}$.

The generator s_α corresponds to the reflection

$$\boxed{s_\alpha : v \to s_\alpha(v) = v - 2\frac{(v|\alpha)}{(\alpha|\alpha)}\alpha}$$

at a hyperplane perpendicular to the root vector α.

The action of the Coxeter group is to permute these root vectors.

Affine extensions

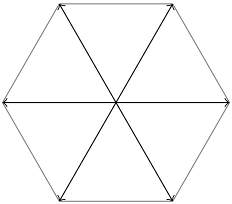
An affine Coxeter group is the extension of a Coxeter group by an affine reflection in a hyperplane not containing the origin $s_{\alpha_0}^{aff}$ whose geometric action is given by

$$\boxed{s_{\alpha_0}^{aff} v = \alpha_0 + v - \frac{2(\alpha_0|v)}{(\alpha_0|\alpha_0)}\alpha_0}$$

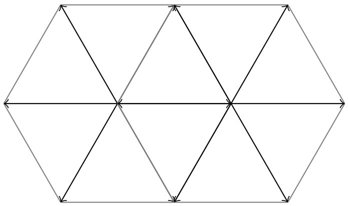
Non-distance preserving: includes the translation generator

$$\boxed{Tv = v + \alpha_0 = s_{\alpha_0}^{aff} s_{\alpha_0} v}$$

Affine extensions – A_2

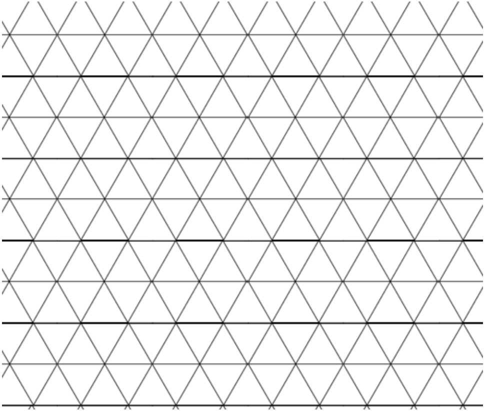


Affine extensions – A_2

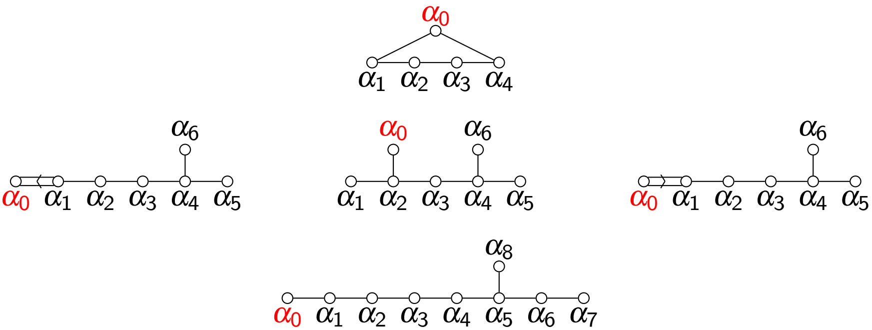


Affine extensions – A_2

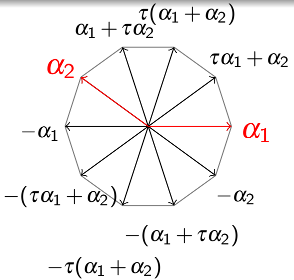
Affine extensions of crystallographic Coxeter groups lead to a tessellation of the plane and a lattice.

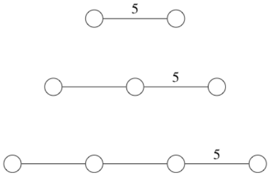


Affine extensions of crystallographic groups A_4, D_6 and E_8



Non-crystallographic Coxeter groups $H_2 \subset H_3 \subset H_4$





$$A = \begin{pmatrix} 2 & -\tau \\ -\tau & 2 \end{pmatrix}$$

$$A = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -\tau \\ 0 & -\tau & 2 \end{pmatrix}$$

$$A = \begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$H_2 \subset H_3 \subset H_4$: 10, 120, 14,400 elements, the only Coxeter groups that generate rotational symmetries of order 5

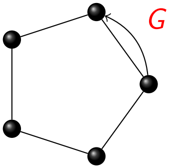
linear combinations now in the extended integer ring

$$\boxed{\mathbb{Z}[\tau] = \{a + \tau b | a, b \in \mathbb{Z}\}}$$ golden ratio $$\boxed{\tau = \frac{1}{2}(1+\sqrt{5}) = 2\cos\frac{\pi}{5}}$$

$$\boxed{x^2 = x + 1} \quad \boxed{\tau' = \sigma = \frac{1}{2}(1-\sqrt{5}) = 2\cos\frac{2\pi}{5}} \quad \boxed{\tau + \sigma = 1, \tau\sigma = -1}$$

Affine extensions of non-crystallographic root systems

Unit translation along a vertex of a unit pentagon



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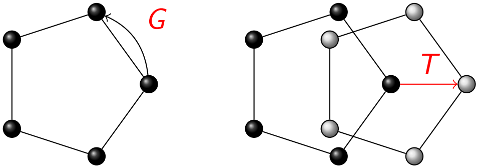

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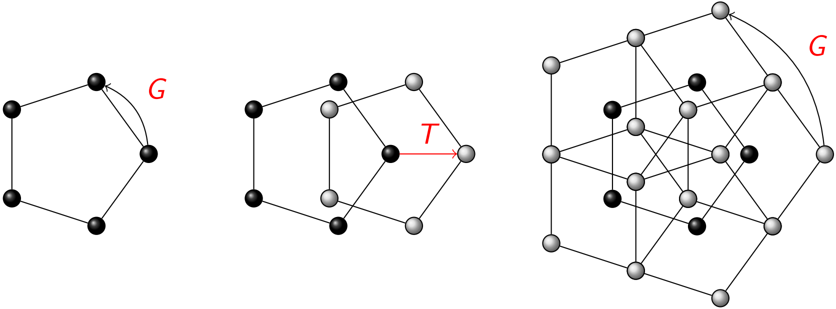
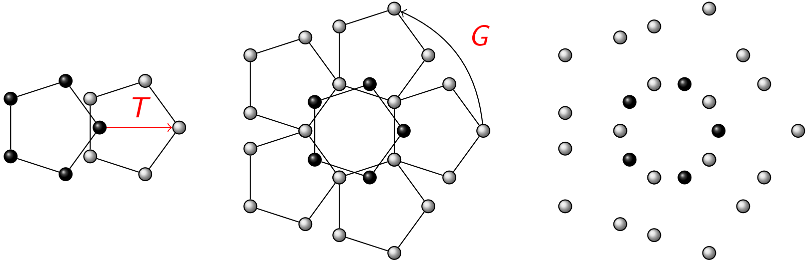


A random translation would give 5 secondary pentagons, i.e. 25 points. Here we have degeneracies due to 'coinciding points'.

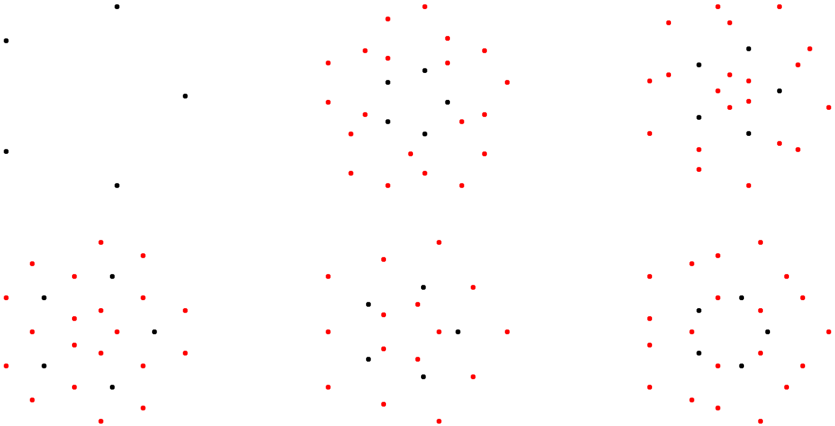
Affine extensions of non-crystallographic root systems

Translation of length $\tau = \frac{1}{2}(1+\sqrt{5}) \approx 1.618$ (golden ratio)



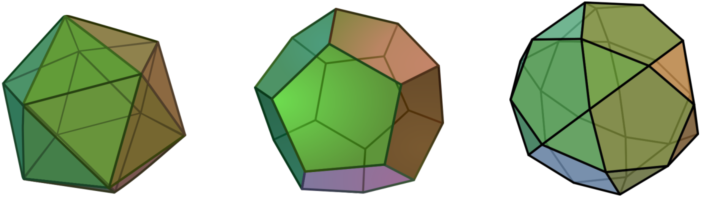
Looks like a virus or carbon onion

More Blueprints

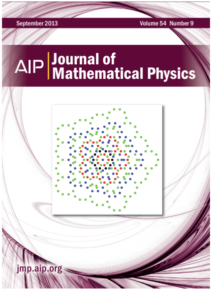


Extend icosahedral group with distinguished translations

- Radial layers are simultaneously constrained by affine symmetry
- Affine extensions of the icosahedral group (giving translations) and their classification.

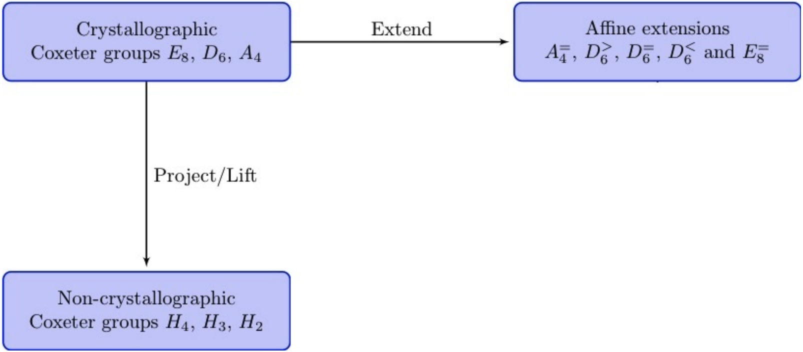


Applications of affine extensions of non-crystallographic root systems



There are interesting applications to quasicrystals, viruses or carbon onions later, concentrate on the mathematical aspects for now

Road Map


Crystallographic
Coxeter groups E_8, D_6, A_4
Extend
Affine extensions
$A_4^=$, $D_6^>$, $D_6^=$, $D_6^<$ and $E_8^=$
Project/Lift
Non-crystallographic
Coxeter groups H_4, H_3, H_2

Road Map

$$
\begin{tikzcd}
\begin{array}{c}\text{Crystallographic}\\ \text{Coxeter groups } E_8,\ D_6,\ A_4\end{array} \arrow[r, "\text{Extend}"] \arrow[d, "\text{Project/Lift}"] & \begin{array}{c}\text{Affine extensions}\\ A_4^=,\ D_6^>,\ D_6^=,\ D_6^< \text{ and } E_8^=\end{array} \arrow[d, dashed, "\text{Induce (DBT2)}"] \\
\begin{array}{c}\text{Non-crystallographic}\\ \text{Coxeter groups } H_4,\ H_3,\ H_2\end{array} \arrow[r, "\text{Extend (DBT1)}"] & \begin{array}{c}\text{Affine extensions}\\ H_2^=,\ H_3^>,\ H_3^=,\ H_3^< \text{ and } H_4^=\end{array}
\end{tikzcd}
$$

Kac-Moody approach

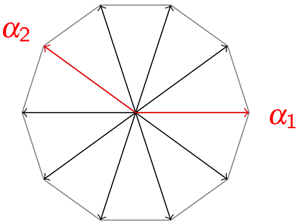
Can recover these directly at the Cartan matrix level:
Kac-Moody-type affine extension A^{aff} of a Cartan matrix is an extension of the Cartan matrix A of a Coxeter group by further rows $\underline{v}$ and columns $\underline{w}$ such that:

$$A^{aff} = \begin{pmatrix} 2 & \underline{v}^T \\ \underline{w} & A \end{pmatrix} \quad \boxed{A^{aff}_{ii} = 2} \boxed{A^{aff}_{ij} \in \mathbb{Z}[\cdot]}$$

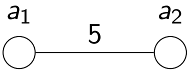
$$\boxed{A^{aff}_{ij} \leq 0} \text{ moreover, } \boxed{A^{aff}_{ij} = 0 \Leftrightarrow A^{aff}_{ji} = 0}$$

determinant constraint $\boxed{\det A^{aff} = 0}$

Kac-Moody approach to H_2

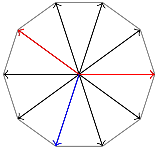


$$\boxed{\alpha_1 = (1,0),\ \alpha_2 = \frac{1}{2}(-\tau, \sqrt{3-\tau})}$$



$$A = \begin{pmatrix} 2 & \cdot & \cdot \\ \cdot & 2 & -\tau \\ \cdot & -\tau & 2 \end{pmatrix}$$

Extension along the highest root

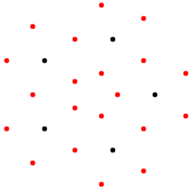


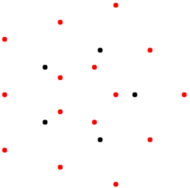
$$A = \begin{pmatrix} 2 & x & x \\ y & 2 & -\tau \\ y & -\tau & 2 \end{pmatrix}$$

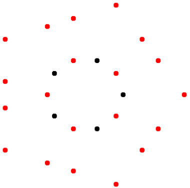
$$\boxed{xy = 2 - \tau = \sigma^2}$$

symmetric $\boxed{x = y = \sigma = 1 - \tau}$ recovers H_2^{aff} from Twarock et al

new asymmetric e.g. $\boxed{(x,y) = (\tau - 2, -1)}$ or $\boxed{(x,y) = (-1, \tau - 2)}$







Write $x = (a + \tau b)$ and $y = (c + \tau d)$ with $a, b, c, d \in \mathbb{Z}$, i.e. H_2^{aff} is $(a, b; c, d) = (1, -1; 1, -1)$.

Fibonacci scaling

The (non-trivial) units in $\mathbb{Z}[\tau]$ are τ^k, $k \in \mathbb{Z}$

Can generate all solutions to the determinant constraint $\boxed{xy = \sigma^2}$ by

scaling $\boxed{x \to \tau^{-k} x, y \to \tau^k y}$: xy invariant (giving the angle),

but different lengths $\sqrt{\frac{x}{y}} \to \sqrt{\frac{x}{y}}\tau^{-k}$

Fibonacci scaling

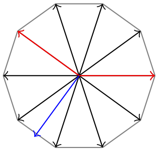
$(a, b; c, d) \to (b, a+b; d-c, c)$ for multiplication by (τ, τ^{-1}) and

$(a, b; c, d) \to (b-a, a; d, c+d)$ for multiplication by (τ^{-1}, τ)

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

Swapping $\boxed{x \leftrightarrow y}$ generates another solution, but here symmetric

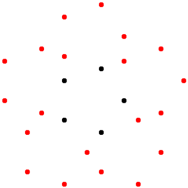
Extension along a bisector

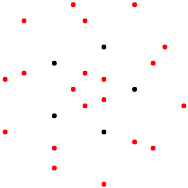


$$A = \begin{pmatrix} 2 & x & 0 \\ y & 2 & -\tau \\ 0 & -\tau & 2 \end{pmatrix}$$

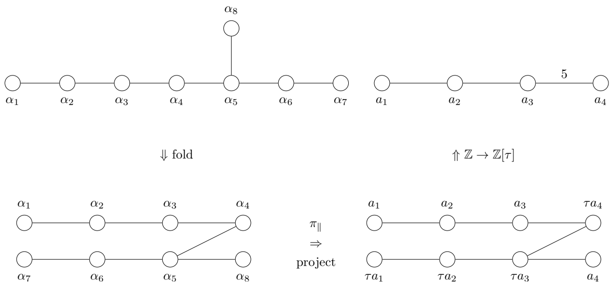
$$\boxed{xy = 3 - \tau}$$

$$\boxed{(x, y) = (\tau - 3, -1)} \text{ or } \boxed{(x, y) = (-1, \tau - 3)}$$





Projection and Diagram Foldings



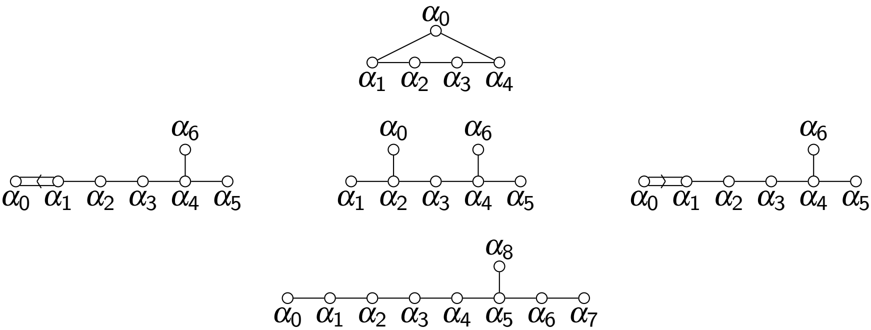
$$\boxed{s_{\beta_1} = s_{\alpha_1} s_{\alpha_7}, \ s_{\beta_2} = s_{\alpha_2} s_{\alpha_6}, \ s_{\beta_3} = s_{\alpha_3} s_{\alpha_5}, \ s_{\beta_4} = s_{\alpha_4} s_{\alpha_8} \Rightarrow H_4}$$

E_8 has two H_4-invariant subspaces – blockdiagonal form

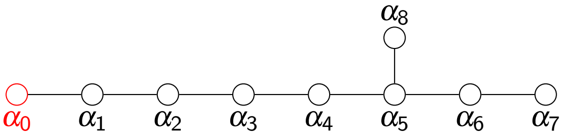
D_6 has two H_3-invariant subspaces

A_4 has two H_2-invariant subspaces

Recap: Affine extensions of crystallographic groups



Affine extensions – $E_8^=$

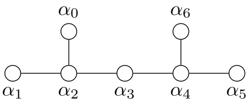


$$\boxed{-\alpha_0 = 2\alpha_1 + 3\alpha_2 + 4\alpha_3 + 5\alpha_4 + 6\alpha_5 + 4\alpha_6 + 2\alpha_7 + 3\alpha_8}$$

AKA E_8^+ and along with E_8^{++} and E_8^{+++} thought to be the underlying symmetry of String and M-theory

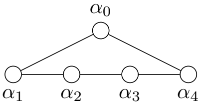
Also interesting from a pure mathematics point of view: E_8 lattice, McKay correspondence and Monstrous Moonshine.

Affine extensions – simply-laced $D_6^=$, $A_4^=$



$$A\left(D_6^=\right) = \begin{pmatrix} 2 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$

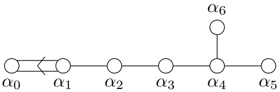
$$\boxed{-\alpha_0 = \alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6}$$



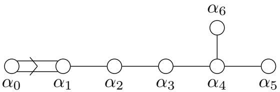
$$A\left(A_4^=\right) = \begin{pmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{pmatrix}$$

$$\boxed{-\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4}$$

Affine extensions – $D_6^<$ and $D_6^>$



$$A\left(D_6^<\right)=\begin{pmatrix} 2 & -2 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$



$$A\left(D_6^>\right)=\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ -2 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$

$$\boxed{-\alpha_0=\alpha_1+\alpha_2+\alpha_3+\alpha_4+\frac{1}{2}\alpha_5+\frac{1}{2}\alpha_6}$$

$$\boxed{-\alpha_0=2\alpha_1+2\alpha_2+2\alpha_3+2\alpha_4+\alpha_5+\alpha_6}$$

Induced affine roots: $H_4^=$ from $E_8^=$

$$\boxed{-\alpha_0 = 2\alpha_1 + 3\alpha_2 + 4\alpha_3 + 5\alpha_4 + 6\alpha_5 + 4\alpha_6 + 2\alpha_7 + 3\alpha_8}$$

$$\boxed{-a_0 = \pi_\parallel(-\alpha_0) = 2(1+\tau)a_1 + (3+4\tau)a_2 + 2(2+3\tau)a_3 + (3+5\tau)a_4}$$

$$\boxed{(a_1|a_2) = -\frac{1}{2},\ (a_2|a_3) = -\frac{1}{2},\ (a_3|a_4) = -\frac{\tau}{2}},$$

$$A(H_4^=) := \begin{pmatrix} 2 & \tau-2 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -\tau \\ 0 & 0 & 0 & -\tau & 2 \end{pmatrix}$$

induced affine root of lengths τ and $1/\tau$ along the highest root $\alpha_H = (1,0,0,0)$ of H_4

Induced affine extensions: $H_i^=$ from $A_4^=$, $D_6^=$ and $E_8^=$

affine extensions of lengths τ and $1/\tau$ along the highest root α_H of H_i

$$A(H_4^=) := \begin{pmatrix} 2 & \tau-2 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -\tau \\ 0 & 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$A(H_3^=) := \begin{pmatrix} 2 & 0 & \tau-2 & 0 \\ 0 & 2 & -1 & 0 \\ -1 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$A(H_2^=) := \begin{pmatrix} 2 & \tau-2 & \tau-2 \\ -1 & 2 & -\tau \\ -1 & -\tau & 2 \end{pmatrix}$$

Induced affine extensions: three H_3^+ from D_6^+

$$A(H_3^=) := \begin{pmatrix} 2 & 0 & \tau-2 & 0 \\ 0 & 2 & -1 & 0 \\ -1 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$A(H_3^<) := \begin{pmatrix} 2 & \frac{4}{5}(\tau-3) & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$A(H_3^>) := \begin{pmatrix} 2 & \frac{2}{5}(\tau-3) & 0 & 0 \\ -2 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

Comparison with DBT1

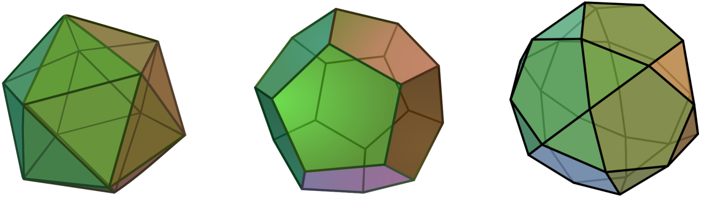
- H_i^{aff} was the symmetric special case of the Fibonacci 'family' of solutions
- $H_i^{=}$ induced by projection of the affine extensions $E_8^{=}$, $D_6^{=}$, $A_4^{=}$ is the 'first asymmetric case'
- Achieved by scaling the symmetric solution of H_i^{aff} by (τ, τ^{-1})
- Projection from $D_6^{<}$ and $D_6^{>}$ give extensions along 5-fold axes of icosahedral symmetry, from $D_6^{=}$ along 2-fold axes
- These are exactly what we were looking for for icosahedral applications!

Overview

1. Affine extensions
   - Direct extensions
   - Induced extensions
2. Applications
   - Virus Structure
   - Fullerenes and Carbon onions
3. Conclusions

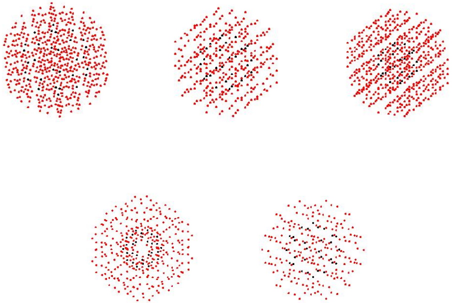
Extend icosahedral group with distinguished translations

- Radial layers are simultaneously constrained by affine symmetry
- Works very well in practice: finite library of blueprints
- Select blueprint from the outer shape (capsid)
- Can predict inner structure (nucleic acid distribution) of the virus from the point array



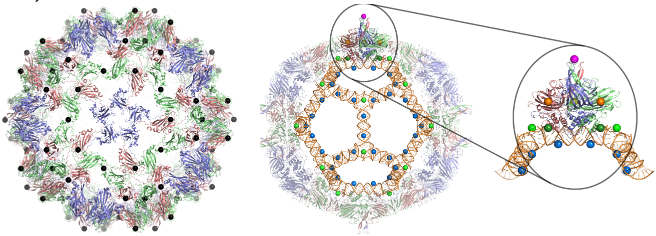
Affine extensions of the icosahedral group (giving translations) and their classification.

What's the point?



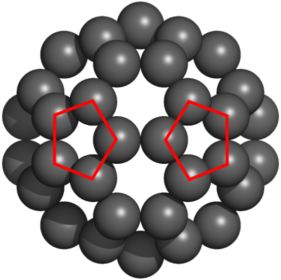
Use in Mathematical Virology

- Suffice to say point arrays work very exceedingly well in practice.
- Implemented computational problem in Clifford algebra – some very interesting mathematics comes out as well (see later).



Constraints of carbon chemistry

- Relevant carbon bonding here is trivalent
- Bond lengths and angles need to be pretty uniform
- For example, the well-known football-shaped Buckyball C_{60}

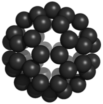


Strategy

- Extend icosahedral shapes with a translation and take orbit under the compact group
- Select outer shells that are three-coordinated and uniform enough
- For the usual icosahedron, dodecahedron, icosidodecahedron find few not very interesting possibilities
- For C_{60} and C_{80} start, get a unique extension that exactly give the known carbon onions $C_{60} - C_{240} - C_{540}$ and $C_{80} - C_{180} - C_{320}$

Fullerene cages derived from C_{60}

- Extend idea of affine symmetry to other objects in nature: icosahedral fullerenes
- Recover different shells with icosahedral symmetry from affine approach starting with C_{60}: carbon onion $(C_{60} - C_{240} - C_{540})$



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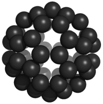

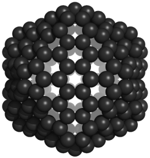

Fullerene cages derived from C_{60}

- Extend idea of affine symmetry to other objects in nature: icosahedral fullerenes
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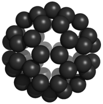
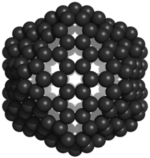
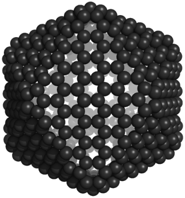
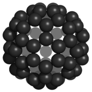






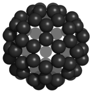
Fullerene cages derived from C_{80}

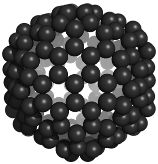
- Extend idea of affine symmetry to other objects in nature: icosahedral fullerenes
- Recover different shells with icosahedral symmetry from affine approach starting with C_{80}: carbon onion $(C_{80} - C_{180} - C_{320})$



Fullerene cages derived from C_{80}

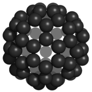
- Extend idea of affine symmetry to other objects in nature: icosahedral fullerenes
- Recover different shells with icosahedral symmetry from affine approach starting with C_{80}: carbon onion $(C_{80} - C_{180} - C_{320})$

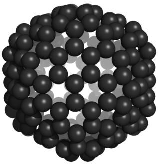


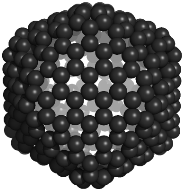


Fullerene cages derived from C_{80}

- Extend idea of affine symmetry to other objects in nature: icosahedral fullerenes
- Recover different shells with icosahedral symmetry from affine approach starting with C_{80}: carbon onion ($C_{80} - C_{180} - C_{320}$)

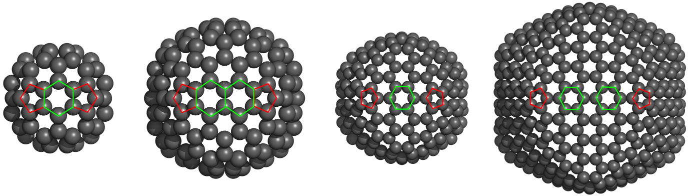






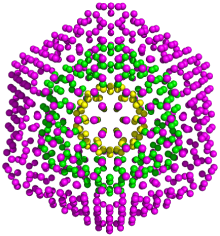
Growth of shells by a hexamer at a time

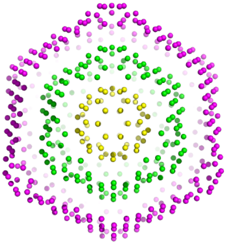
- Hence, for C_{60} and C_{80} start, get a unique extension that exactly give the known carbon onions $C_{60} - C_{240} - C_{540}$ and $C_{80} - C_{180} - C_{320}$ by inserting an additional hexamer at each step



Viruses and fullerenes – symmetry as a common thread?

- Get nested arrangements like Russian dolls: fullerene carbon onions
- Potential to extend to other known carbon onions with different start configuration, chirality etc





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- Affine extensions of non-crystallographic Coxeter groups induced by projection with Twarock/Bœhm Journal of Mathematical Physics 54 093508 (2013), Cover article September
- Viruses and Fullerenes – Symmetry as a Common Thread? with Twarock/Wardman/Keef Acta Crystallographica A 70 (2). pp. 162-167 (2014), Cover article March

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  Advances in Applied Clifford Algebras 23 (2). pp. 301-321 (2013)
- A Clifford algebraic framework for Coxeter group theoretic computations (Conference Prize at AGACSE 2012)
  Advances in Applied Clifford Algebras 24 (1). pp. 89-108 (2014)
- Nomination for W.K. Clifford Prize (2014)
- 6 month invitation to Arizona State University
- Rank-3 root systems induce root systems of rank 4 via a new Clifford spinor construction arXiv:1207.7339 (2012)
- Platonic Solids generate their 4-dimensional analogues
  Acta Cryst. A69 (2013)

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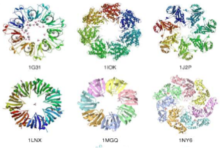
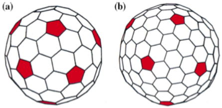
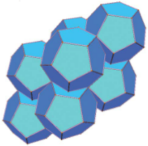
Conclusions

- Novel mathematical structures
- Interesting in their own right
- Numerous applications to real systems: Viruses, Proteins, Fullerenes, Quasicrystals, Tilings, Packings etc.



Thank you!

Extension along the highest root – two-fold axis T_2

$$\boxed{\alpha_1=(0,1,0),\ \alpha_2=-\frac{1}{2}(-\sigma,1,\tau),\ \alpha_3=(0,0,1)}$$

$$\boxed{T_2=(1,0,0)} \qquad A=\begin{pmatrix}2&0&x&0\\0&2&-1&0\\y&-1&2&-\tau\\0&0&-\tau&2\end{pmatrix} \qquad \boxed{xy=\sigma^2=2-\tau}$$

Same solution as in the previous case of H_2.

Extension along a three-fold axis T_3

$$\boxed{\alpha_1 = (0,1,0),\ \alpha_2 = -\frac{1}{2}(-\sigma,1,\tau),\ \alpha_3 = (0,0,1)}$$

$$\boxed{T_3 = (\tau,0,\sigma)} \qquad A = \begin{pmatrix} 2 & 0 & 0 & x \\ 0 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ y & 0 & -\tau & 2 \end{pmatrix} \qquad \boxed{xy = \frac{4}{3}\sigma^2}$$

No longer $\mathbb{Z}[\tau]$-valued, and hence solutions do not exist in $\mathbb{Z}[\tau]$.
What now? Allow $\mathbb{Q}[\tau]$? Write $x = \gamma(a+\tau b)$ and $y = \delta(c+\tau d)$ with $a,b,c,d \in \mathbb{Z}$ and $\gamma,\delta \in \mathbb{Q}$. Need $\boxed{\gamma\delta = \frac{4}{3}}$, then can recycle integer solution

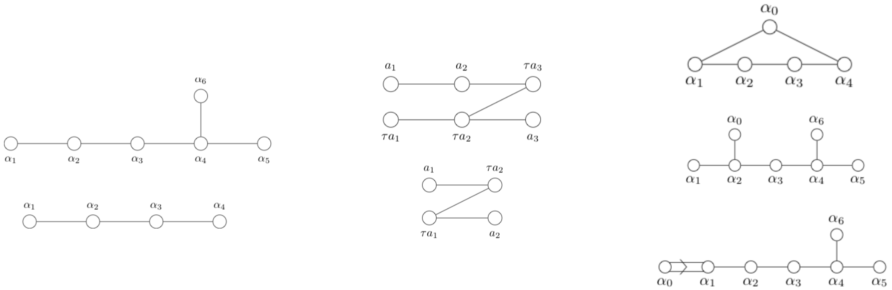
Extension along a five-fold axis T_5

$$\boxed{\alpha_1 = (0,1,0),\ \alpha_2 = -\frac{1}{2}(-\sigma,1,\tau),\ \alpha_3 = (0,0,1)}$$

$$\boxed{T_5 = (\tau,-1,0)} \qquad A = \begin{pmatrix} 2 & x & 0 & 0 \\ y & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix} \qquad \boxed{xy = \frac{4}{5}(3-\tau)}$$

Same solution (two series) as before in the case of H_2, but this time with the additional degree of freedom.

Invariance under Dynkin diagram automorphisms



$$\boxed{-\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4}$$

$$\boxed{-\alpha_0 = \alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6}$$

$$\boxed{-\alpha_0 = 2\alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6}$$